Analyzing the spectrum of general, non-hermitian Dirac operators

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We discuss the computational problems when analyzing general, non-hermitian matrices and in particular the un-modified Wilson lattice Dirac operator. We report on our experiences with the Implicitly Restarted Arnoldi Method. The eigenstates of the Wilson-Dirac operator which have real eigenvalues and correspond to zero modes in the continuum are analyzed by correlating the size of the eigenvalues with the chirality of the eigenstates.

1. THE PROBLEM

Analyzing the eigensystem of large matrices such as the Dirac operator in 4-D lattice field theory is a quite demanding numerical task. Furthermore the lattice Dirac operator in Wilson formulation is neither hermitian nor anti-hermitian which poses an additional difficulty compared to a case with symmetry.

The Wilson-Dirac operator consists of a trivial part (proportional to the unit matrix) which comes from mass- and Wilson terms and a non-trivial part K. Here we analyze the clover-improved [1] Wilson-Dirac operator and K consists of two parts $K = Q - c_{sw}C$ where Q is the standard Wilson hopping matrix and C the clover term. The matrix K is neither hermitian nor anti-hermitian, but hermitian conjugation is implemented through the similarity transformation

$$\gamma_5 K \gamma_5 = K^\dagger . \qquad (1)$$

The relation (1) allows to define the hermitian modification $\gamma_5 K$ and several numerical studies of this modified matrix can be found in the literature. For a deeper understanding of the lattice Dirac operator however one would also like to study the original problem.

2. THE IMPLICITLY RESTARTED ARNOLDI METHOD

The two main techniques to solve large scale eigenvalue problems are Krylov subspace methods: The Lanczos algorithm, which transforms the original matrix to tridiagonal form, or, in the case of non-hermitian matrices, the Arnoldi method, which transforms to Hessenberg form. Since typically the Hessenberg form is dense it is necessary to compress the relevant information in a Krylov subspace of small dimension. This can be done by using the Implicitly Restarted Arnoldi Method (IRAM) [2]. IRAM has several favorable features: The numerical precision is comparable to dense methods, IRAM is able to find degeneracies and it gives both eigenvalues and eigenvectors. The software package ARPACK with an efficient and reliable implementation of the IRAM was developed by Sorensen and collaborators [3]. The method turns out to be particularly useful when analyzing the edges of the spectrum. It can e.g. be set up such that the eigenvalues with largest real parts are computed first. This gives the eigenvalues in the physical branch of the spectrum. In Fig. 1 we show the physical branch of the spectrum in the complex plane for a thermalized SU(2) gauge field configuration $(12^4, \beta = 2.4, c_{sw} = 1.4)$ and compare it to its cooled counterpart $(c_{sw} = 1)$. Both gauge field configurations were taken from [4].
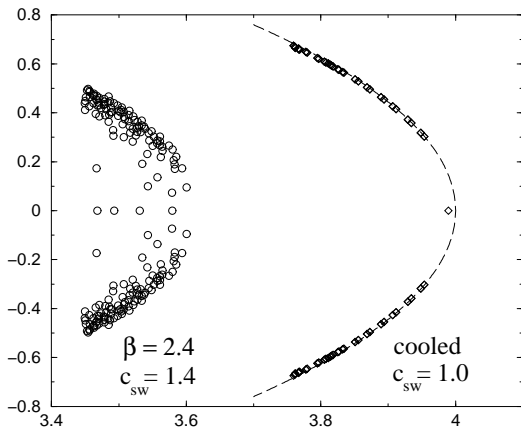
Figure 1. Physical branch of the spectrum of K for a thermalized configuration and its cooled counterpart.

As is obvious from the plot cooling leads to a strong shift of the eigenvalues and orders them along a single curve (ellipse). What is also interesting to note is the fact that the thermalized configuration has considerably more real eigenvalues in the physical branch than its cooled counterpart. In [5] it was shown, that these additional real eigenvalues are partly due to the clover term. This proliferation of real eigenvalues makes a probabilistic interpretation of the Atiyah-Singer index theorem for thermalized configurations problematic, as will be discussed in the next section.

For a complete understanding of the properties of the lattice Dirac operator it is also interesting to analyze eigenvalues in the interior of the spectrum, in particular on the real axis. However, as with all Krylov subspace methods, the convergence of the interior eigenvalues is very slow and one has to use some kind of spectral preconditioning. Traditionally, to find the eigenvalues in the vicinity of some point z in the complex plane a shift of the origin is combined with inversion, i.e. the eigenvalues of $(K - z\mathbb{1})^{-1}$ are searched for. This requires solving a large linear system at every iteration which makes this approach quite inefficient. However, for matrices which satisfy (1) a kind of sophisticated preconditioning can be used [6]. The shift of the origin is combined

with a multiplication with γ_5 to transform the original non-hermitian to a hermitian eigenvalue problem. Although the explicit relation between eigenvalues of original and transformed matrix is not known the zero eigenvalues and their eigenvectors are the same. By shifting the origin along the real axis, it is possible to identify real eigenvalues. In particular one traces the flow of low lying eigenvalues of $H(\rho) \equiv \gamma_5[K - \rho\mathbb{1}]$ as a function of ρ. Whenever the flow crosses zero at some $\rho = r$, then this r is a real eigenvalue of K. The chirality of the mode can be computed from the slope of the eigenvalue flow at the crossing. Even for this hermitian problem we found the IRAM method superior (numerical stability, precision and efficiency) to our implementation of the accelerated conjugate gradient algorithm [7] which is usually used for this purpose. Further gain in efficiency can be achieved by using Chebyshev polynomials to project out the desired part of the spectra.

3. SOME RESULTS ON THE REAL PART OF THE SPECTRUM

It was already remarked that the real eigenvalues of the lattice Dirac operator are of particular interest. This is a consequence of (1) which implies that $\psi^\dagger \gamma_5 \psi$ is different from 0 only for eigenvectors ψ of the Dirac operator which have real eigenvalues. Thus a comparison of the chiral properties of the eigenstates implies that only eigenvectors with real eigenvalues can play the role of the zero modes in the continuum [6,8]. Based on this interpretation of the eigenvectors with real eigenvalues as the lattice zero modes one can formulate a lattice version of the Atiyah-Singer index theorem: $\nu[U] = R_- - R_+$. Here R_+ and R_- are the numbers of real eigenvalues in the physical branch of the spectrum with positive and negative chirality. The chirality is defined as the sign of the pseudoscalar matrix element of the corresponding eigenvectors and $\nu[U]$ denotes the topological charge of the gauge field.

The lattice version of the index theorem is expected to hold for sufficiently smooth gauge field configurations. This was demonstrated for smooth SU(2) and SU(3) background configura-

tions [9] and for fully quantized QED_2 [10]. For thermalized SU(2) and SU(3) configurations the situation is less clear [5,6,11]. There is no one-to-one corespondence [5] between the value of the topological charge assigned using the index theorem and the value from improved cooling [4] and only averaging over larger samples or studying density functions of eigenvalues [11] allows a probabilistic interpretation of the index theorem.

Here[2] we correlate the position of the real eigenvalues with the size of the pseudoscalar matrix element $\psi^\dagger \gamma_5 \psi$ for the corresponding eigenvectors ψ. For smooth gauge field configurations the real eigenvalues in the physical branch of K are in the vicinity of 4 on the real axis and the pseudoscalar matrix elements are in the vicinity of ± 1, the sign given by the chirality of the mode. For thermalized configurations the absolute value of the pseudoscalar matrix elements becomes smaller and additional pairs of real eigenvalues with opposite chirality are created [5]. We check if the artificial real eigenvalues from the clover term have smaller pseudoscalar matrix elements and if this can be used to discriminate between the would-be zero modes on the lattice and the additional real modes. In Fig. 2 we show a scatter plot containing the eigenvalues between 1.8 and 4 on the real axis using a sample of 10 thermalized gauge field configurations ($12^4, \beta = 2.4, c_{sw} = 1.4$). The horizontal axis gives their position on the real axis and on the vertical axis we plot the pseudoscalar matrix elements of the corresponding eigenvectors.

If there was a clear separation of the lattice would-be zero modes from artificial real modes (due to strongly fluctuating fields and the clover term) one would find two well isolated islands of points in the upper and lower right corners of our plot. However, as is clear from the figure no such separated islands exist and we have to close with the conclusion of [5] that for $12^4, \beta = 2.4, c_{sw} = 1.4$ there is no proper separation between physical zero modes and artifacts.
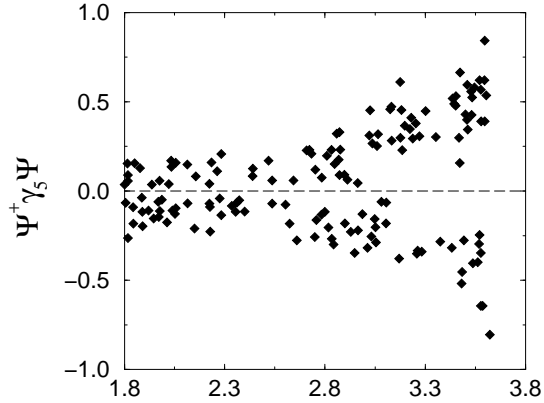
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[2]We thank P. de Forcrand for suggesting to analyze the correlation with the pseudoscalar matrix elements.

Figure 2. Correlation of the real eigenvalues with the corresponding pseudoscalar matrix elements.

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